A Class of Self-Trapped and Self-Focusing Wave Functions in Madelung Fluid Picture of A Single Free Particle Quantum System

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Abstract

Using the Madelung fluid picture of Schrödinger equation for a single free particle moving in one spatial dimension, we shall specify a class of wave functions whose quantum probability density is being trapped by the quantum potential it itself generates. The global convexity of the quantum potential generated by the initial self-trapped wave function will then be shown to further localize the quantum probability density through a self-generated focusing equation for a finite interval of time.

Key words: single free particle quantum system; Madelung fluid;

self-trapped wave function *PACS*: 03.65.Ge; 03.65.Ca

1. Motivation: Schrödinger Equation as Self-Referential Dynamics

Let us consider a quantum system of a single free particle with mass m moving in one dimensional space, q. The wave function $\psi(q;t)$, where t is time, is then governed by the linear Schrödinger equation

$$i\hbar\partial_t\psi(q;t) = -\frac{\hbar^2}{2m}\partial_q^2\psi(q;t).$$
 (1)

Quantum theory claims that the quantum probability density, $\rho(q) = |\psi(q)|^2$, gives the essential information about the position of the particle [1, 2, 3, 4]. Hence, it is important to study the dynamics of $\rho(q;t)$.

One way to keep track directly the dynamics of $\rho(q;t)$ is to use Madelung fluid hydrodynamical interpretation of the Schrödinger equation [5]. To do

this, let us write the wave function in polar form, $\psi(q;t) = R(q;t) \exp(iS(q;t)/\hbar)$, where the quantum amplitude R and the quantum phase S are real-valued functions. Inserting this into Eq. (1) and separating the real and imaginary parts, one gets

$$\partial_t S + \frac{(\partial_q S)^2}{2m} + U = 0,$$

$$\partial_t \rho + \partial_q \left(\frac{\partial_q S}{m} \rho\right) = 0,$$
(2)

where U is the so-called quantum potential generated by the quantum probability density as

$$U(q;t) = -\frac{\hbar^2}{2m} \frac{\partial_q^2 R}{R}.$$
 (3)

Next, let us define a velocity field as

$$v(q;t) = \frac{1}{m} \partial_q S(q;t). \tag{4}$$

Taking the spatial gradient to both sides of the upper equation in (2), and using Eq. (4) one has

$$m\frac{dv}{dt} = -\partial_q U. (5)$$

Due to its similarity with Euler equation, the term on the right hand side of the above equation, $-\partial_q U$, is usually called as quantum force field. Moreover, again using Eq. (4), the lower equation in (2) can be seen as the continuity equation for $\rho(q;t)$.

One of the great lesson from the Madelung fluid picture is its self-referential property. Namely, the quantum probability density $\rho(q;t)$ will generate a quantum potential U(q;t) which in turn will rule the quantum probability density the way it must flow and so on and so forth. There is a dynamics circularity between the object to be ruled and the rule itself. Self-referential property is a simpton of complex non-linear systems, and is argued to be the general origin for the emergence of many interesting phenomena [6]. We can then expect to find interesting self-organized behavior difficult to be observed directly from Eq. (1), at least in a certain time scale.

To see an example of the effect of the self-referential property of the Madelung fluid and to help describing the motivation of the present work,

let us discuss the dynamics of a Gaussian wave packet. In this case the quantum probability density will take the form [7]

$$\rho(q;t) = \frac{1}{Z} \exp\left(-\frac{q^2}{2\sigma_t^2}\right), \ \sigma_t^2 = \sigma^2 + \frac{\hbar^2 t^2}{4m^2 \sigma^2}.$$
 (6)

Here, Z is the trivial normalization constant, σ_t is the width of the wave packet at time t and σ is its width at t = 0. The corresponding quantum potential can thus be calculated to give

$$U(q;t) = -\frac{\hbar^2 q^2}{8m\sigma_t^2} + \frac{\hbar^2}{4m\sigma_t}.$$
 (7)

One can clearly see from the global concavity of the quantum potential given above that the quantum force field is repelling the quantum probability density to spread out. As time goes, the quantum probability density keeps its Gaussian form but is rescaled to be wider. This will also rescale the quantum potential to be wider while keeping its form, thus keeps the effect of repelling the quantum probability density. This simple picture is missing in the original Schrödinger equation of (1). Hence, Gaussian wave packet provides an example of a class of wave functions being repelled by its own self-generated quantum potential.

The question that we want to discuss in this paper is then: is there any class of wave functions whose quantum probability density is self-trapped or self-attracted by the quantum potential it itself generates?

2. Self-Trapped quantum probability density

Obviously, the self-trapped quantum probability density that we want to develop must decay as the self-generated quantum potential increases. One therefore has to develop another relation between ρ and U which provides the supplement to Eq. (3). There are many possibilities to create an $\rho - U$ relation which satisfies the above mentioned condition. In this paper, we shall consider a class of wave functions $\{\psi\}$, whose quantum probability density is given as the exponential of its quantum potential as follows

$$\rho(q;t) = \frac{1}{Z(\beta)} \exp\left(-\beta U(q;t)\right),\tag{8}$$

where β is a positive real-valued contant, and Z is a normalization factor given by $Z = \int dq \exp(-\beta U)$. It is then clear that ρ decays as U grows.

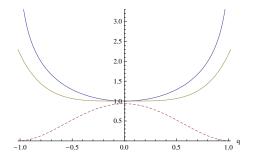


Figure 1: The profile of quantum potential U(q) (solid blue line) satisfying Eq. (9), and the corresponding quantum probability density $\rho(q)$ (dashed line) which generates the quantum potential. The solid red curve is the approximation of U(q) given by Eq. (11).

Notice that Eq. (8) together with the definition of quantum potential given in Eq. (3) comprise a differential equation for $\rho(q)$ or U(q), subjected to the condition that $\rho(q)$ must be normalized.

In term of U, taking the spatial derivative twice to both sides of Eq. (8) and recalling the definition of quantum potential given in Eq. (3) one obtains

$$\partial_q^2 U = \frac{\beta}{2} (\partial_q U)^2 + \Lambda^2 U, \tag{9}$$

where $\Lambda = \sqrt{4m/\hbar^2\beta}$. First, one can see from the above equation that the positivity of quantum potential, U > 0, guarantees its local convexity, $\partial_q^2 U > 0$. Further, it is clear that the above differential equation is invariant under the transformation $q \to -q$. These facts will guide us later to find a class of solutions which are positive everywhere (thus convex everywhere), and symmetric with respect to the vertical line q = 0.

Let us first solve Eq. (9) for a spatial region very close to the extremum points of the quantum probability density or quantum potential, $|q-Q| \ll 1$, where Q is the extremum point under consideration satisfying $\partial_q U(Q) = \partial_q U|_Q = 0$. In this case, assuming the continuity of $\partial_q U$, the first term on the right hand side can be ignored, $\partial_q U \approx 0$. Hence, in this spatial region we have

$$\partial_q^2 U \approx \Lambda^2 U, \quad |q - Q| \ll 1.$$
 (10)

The above differential equation can then be solved with constraint $\partial_q U|_Q = 0$ and $U(Q) = U_Q$, to give

$$U(q) \approx U_Q \cosh\left(\pm \Lambda(q-Q)\right), \quad |q-Q| \ll 1.$$
 (11)

The point Q turns out to be the local minimum (maximum) point of the quantum potential U(q) if U_Q is positive (negative).

To check the desirable trapping property, one must see the global behavior of the quantum probability density and its corresponding quantum potential. To do this one should solve equation Eq. (9) for the whole space. We shall resort to numerical methods to do this. For the reason mentioned previously, we shall confine ourselves to a class of solutions which satisfy the following boundary conditions $\partial_q U|_0 = 0$ and $U_0 > 0$. Namely, we want to find a class of solutions where the first spatial derivative at the origin is vanishing, and let U_0 to varies only to positive values. The first condition will explore the symmetry of the differential equation, while the second boundary condition will guarantee that the quantum potential is nowhere non-convex. Note that the case $U_0 = 0$ is trivial. Namely, imposing the boundary condition $\partial_q U|_0 = 0$ to Eq. (9) one gets $\partial_q^2 U|_0 = 0$ such that U(q) = 0 everywhere. Hence, $\rho(q)$ is unnormalizable. This case therefore is excluded from our consideration. Fig. 1 shows the numerical solution of Eq. (9) with the boundary condition $\partial_q U|_0 = 0$ and $U_0 = 1$. The profile of quantum probability density (dashed line) is plotted together with the profile of quantum potential it itself generates (solid blue line). For comparation, we have also plotted the approximate solution given in Eq. (11) (solid red line).

First, it is observed that very near to the extremum point, q=0, Eq. (11) fits the numerical solution very well. Yet it immediately departs from the numerical solution as |q| is getting larger. We can see clearly from the numerical solution that globally the quantum probability density is indeed being trapped by the quantum potential it itself generates. This global property can be understood for any positive value of $U_0>0$ as follows. First from Eq. (9), inserting the boundary conditions at q=0, one gets $\partial_q^2 U|_0=\Lambda U_0>0$, such that U(q) is locally convex at q=0. Hence, since $\partial_q U|_0=0$, at spatial points nearby q=0 one has $U(q)>U_0>0$. Moreover since the second term on the right hand side of Eq. (9) is always non-negative, at this region one has $\partial_q^2 U>0$. This geometrical reasoning can be extended such that for the whole space one gets

$$\partial_q^2 U > 0. (12)$$

Namely, the case when $U_0 > 0$ will give an everywhere positive and convex quantum potential. Hence, q = 0 turns out to be the global minimum of U(q). Using this fact in Eq. (8) one can conclude that quantum probability density, $\rho(q)$, is being trapped by its own self-generated quantum potential,

U(q).

Next, from the definite positivity of the quantum potential and Eq. (3), one has

$$\partial_a^2 R < 0. (13)$$

Hence, the quantum amplitude is everywhere concave. Supplied with the fact that R(q) is finite, one can conclude that R(q) must cross the q-axis at finite value of $q = \pm q_m$. This means that the support of R(q), $[-q_m, q_m]$ is finite. At $q = \pm q_m$, U(q) is infinite, yet the quantum probability density is vanishing. Further, notice that at $q = \pm q_m$, $\partial_q R(q)$ is discontinuous. However, $\partial_q \rho(q) = 2R(q)\partial_q R(q) = 0$ is continuous. Hence, the self-trapped wave functions is a truly localized wave function with finite tail (support).

Now let us compare the class of self-trapped wave functions we developed in this paper with Gaussian wave packet. As discussed in section 1, the latter represents a class of self-repelled wave functions. Fig. 2 shows a self-trapped quantum probability density (solid line) plotted together with the Gaussian wave packet (dashed line) of the same second moment. One can see that Gaussian is more localized in the region near the maximum. Yet, in contrast to the self-trapped quantum probability density which possesses support only on a finite region, the Gaussian wave packet possesses support on the whole space.

Another interesting difference between Gaussian and self-trapped wave function is that though both are quite similar to each other, their corresponding quantum potentials are very contrast from each other. While the quantum potential generated by Gaussian wave packet is concave everywhere, the quantum potential of self-trapped wave function developed in this paper is convex everywhere. As will be discussed in the next section, one can then expect that this makes their future destiny very different from each other at least for a finite period of time.

3. Self-Generated Focusing Equation

Intuitively, for spatially one dimensional case we are considering, the global convexity of the quantum potential makes the quantum force field to drag the quantum probability density toward the center, *i.e.* the global minimum of the quantum potential, at least for some interval of time. To see this more clearly, let us take the spatial derivative to both sides of Eq. (5) to give us

$$md_t\theta = -m\theta^2 - \partial_q^2 U. (14)$$

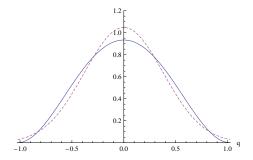


Figure 2: The profile of a self-trapped quantum probability density (solid line) compared with a Gaussian quantum probability density (dashed line) with the same second moment.

Here $d_t \equiv d/dt$, $\theta = \partial_q v = \partial_q^2 S/m$ is the velocity divergence and we have used the following fact from the differential calculus $d_t = \partial_t + v\partial_q$. Hence, for the class of self-trapped wave functions we are considering here, where $\partial_q^2 U > 0$ everywhere, one will get

$$d_t \theta < 0, \tag{15}$$

which is a focusing equation. Let us note that the above relation is valid for any value of $\theta(q)$, hence for any form of quantum phase S(q). One can thus conclude that in contrast to Gaussian wave packet which is self-repelled everywhere, the self-trapped wave function is self-focused everywhere.

Due to the continuity of the evolution of U(q;t) which is guaranteed by the continuity equation in the lower part of (2), U(q;t) will keep its global convexity for a certain finite interval of time, say T. Given an initial selftrapped quantum probability density, $\rho(q;0)$, T of course depends on the initial quantum phase as well. Thus it depends on θ_0 , $T = T(\theta_0)$, where θ_0 is the value of $\theta = (1/m)\partial_q^2 S$ at t = 0. Yet, the finite-ness of T is independent of the choice of θ_0 . Namely, no initial wave function can avoid the focusing equation of (15). In particular, during the interval of time T one has

$$d_t \theta + \theta^2 = -(1/m)\partial_a^2 U \le 0. \tag{16}$$

This will imply $d_t(\theta^{-1}) \geq 1$, such that one obtains

$$\theta^{-1}(t) \ge \theta_0^{-1} + t. \tag{17}$$

The above inequality shows that if θ_0 is negative, then within a time $t_c < 1/|\theta_0|$, θ^{-1} must pass zero, namely, one has $\theta \to -\infty$. Of course this will

occur as long as

$$1/\theta_0 \le T(\theta_0),\tag{18}$$

possesses a solution. Hence, caustics will develop in a finite interval of time. During this time, the quantum probability density keeps converging toward the origin.

4. Conclusion and Discussion

To conclude, first we have specified a class of wave functions whose quantum probability densities are being trapped by the quantum potentials they themselves generate. The self-trapped wave functions are then dragged by a self-generated focusing equation of (15) to localize even further, at least for certain interval of time depending on the initial quantum phase.

For a given initial self-trapped quantum probability density, if there is θ_0 such that inequality (18) is satisfied, then the velocity divergence is equal to minus infinity everywhere, $\theta \to -\infty$, in a finite time. During this period of time, the quantum probability density converges everywhere until caustics is developed. The next question is then to investigate whether the singularity in velocity field (caustic) will also induce a singularity in quantum potential and how the quantum probability density looks like at this time. It is also tempting to study what happens to the wave function after the development of caustics. We leave this for future work.

References

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